10690341

(FILE 'HOME' ENTERED AT 12:22:55 ON 13 NOV 2004)

FILE 'REGISTRY' ENTERED AT 12:23:07 ON 13 NOV 2004
L1 STRUCTURE UPLOADED
L2 STRUCTURE UPLOADED
L3 0 S L1
L4 0 S L2
L5 20 S L2 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:25:40 ON 13 NOV 2004
L6 4 S L5
L7 STRUCTURE UPLOADED
S L7

FILE 'REGISTRY' ENTERED AT 12:30:26 ON 13 NOV 2004
L8 0 S L7

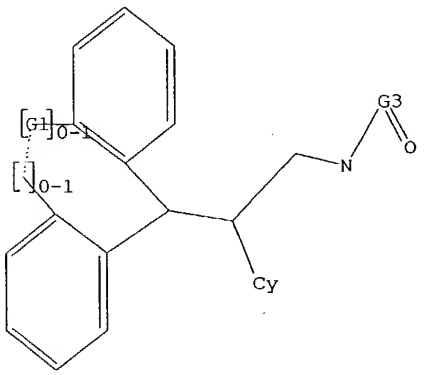
FILE 'CAPLUS' ENTERED AT 12:30:27 ON 13 NOV 2004
L9 0 S L8

FILE 'REGISTRY' ENTERED AT 12:30:40 ON 13 NOV 2004
L10 23 S L7 SSS FULL

FILE 'CAPLUS' ENTERED AT 12:31:14 ON 13 NOV 2004
L11 7 S L10

=> s l11 not l6
L12 4 L11 NOT L6

=> d 12
L2 HAS NO ANSWERS
L2 STR



G1 O,S,N,C

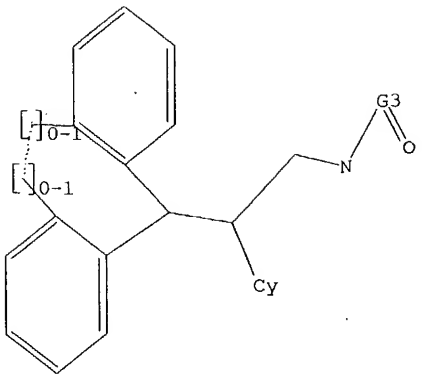
G2

G3 C,S

Structure attributes must be viewed using STN Express query preparation.

=> d l7
L7 HAS NO ANSWERS
L7 STR

10690341



G1 O,S,N,C

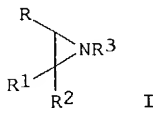
G2

G3 C,S

Structure attributes must be viewed using STN Express query preparation.

=> d 1-4 bib abs hitstr

L12 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1991:655913 CAPLUS
DN 115:255913
TI Nitrogen-sulfur cleavage is faster than homolytic ring opening in single-electron transfer to some N-sulfonylaziridines. Competition between SN2 and SET
AU Bellos, Konstantinos; Stamm, Helmut; Speth, Dieter
CS Pharm.-Chem. Inst., Fac. Pharm., Heidelberg, D-6900, Germany
SO Journal of Organic Chemistry (1991), 56(24), 6846-9
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
GI



I

AB The radical anions of the N-sulfonylaziridines I (R = H, R1 = Ph, CH2Ph, R2 = CMe3, Y = tosyl; R = PhCH2, R1 = Ph, R2 = H, R3 = SO2Ph) undergo N-S cleavage in place of homolytic ring opening upon treatment with Na anthracenide. Nucleophilic ring opening of these sulfonylaziridines by the carbanions of dihydroanthracene, xanthene, and fluorene, resp., proceeds with the expected regioselectivity and is slow enough to allow some competition by a single-electron transfer (SET) initiated N-S cleavage, which provides the desulfonated aziridines and bixanthenyl or bifluorenyl, resp. The SET path is favored by light. The competition is in favor of SET to the exclusion of the nucleophilic opening when trityl anion reacts with I (R = H, R1 = Ph, R2 = CMe3, R3 = tosyl).

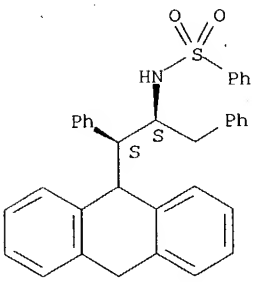
IT **136175-24-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 136175-24-1 CAPLUS

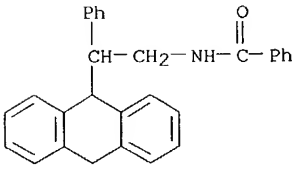
CN Benzenesulfonamide, N-[2-(9,10-dihydro-9-anthracenyl)-2-phenyl-1-(phenylmethyl)ethyl]-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

10690341



L12 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1990:631105 CAPLUS
DN 113:231105
TI Reactions with aziridines. 53. Arene hydrides. 9. Intermediate substitution in the formation of a benzylic anion by an aromatic radical anion as observed with 1-benzoyl-2-phenylaziridine
AU Stamm, Helmut; Falkenstein, Reinhart
CS Pharm. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Germany
SO Chemische Berichte (1990), 123(11), 2227-30
CODEN: CHBEAM; ISSN: 0009-2940
DT Journal
LA English
OS CASREACT 113:231105
AB The reaction of the title compound (I) with anthracene hydride (AH-) or anthracenide (A-•) leads to the formation of the benzylic anion PhCH-CH2N:CPhO- (II) by fragmentation of the first generated substitution intermediate PhCHRCH2N:CPhO- (R = 9,10-dihydroanthracen-9-yl or its 10-anion). In the reactions with AH- the carbanion II is completely trapped by protonation with dihydroanthracene, yielding the reduction product PhCH2CH2NHBz (III). In reactions with A-• as well as with sodium naphthalenide, carbanion II either abstrs. a proton from the solvent (THF) yielding III, or adds to the benzoyl group of unreacted I which finally results in PhCOCHPhCH2NHBz.
IT **128600-81-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive cleavage of, with anthracene hydride)
RN 128600-81-7 CAPLUS
CN Benzamide, N-[2-(9,10-dihydro-9-anthracenyl)-2-phenylethyl]- (9CI) (CA INDEX NAME)



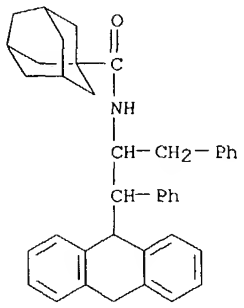
L12 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1989:173013 CAPLUS
DN 110:173013
TI Reductive ring opening of N-benzoylaziridine by anthracene hydride (anion of 9,10-dihydroanthracene) via base-induced fragmentation of the intermediate carbonyl adduct
AU Stamm, Helmut; Mall, Thomas; Falkenstein, Reinhard; Werry, Juergen; Speth, Dieter
CS Pharm. Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.
SO Journal of Organic Chemistry (1989), 54(7), 1603-7
CODEN: JOCEAH; ISSN: 0022-3263
DT Journal
LA English
OS CASREACT 110:173013
AB Reaction of anthracene hydride, or of its oxa analog xanthenyl anion with N-benzoylaziridines I can result in amidoethylation of the carbanion, in reductive opening of the aziridine ring, and in attack on the carbonyl

group I. With I both the rate of ring opening and the amount of reductive opening are significantly enhanced by an excess of 9-lithio-9,10-dihydroanthrocene while the initially formed (90%) carbonyl adduct survives with a deficit of 9-lithio-9,10-dihydroanthrocene.

IT **119297-90-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 119297-90-4 CAPLUS

CN Tricyclo[3.3.1.13,7]decane-1-carboxamide, N-[2-(9,10-dihydro-9-anthracenyl)-2-phenyl-1-(phenylmethyl)ethyl]-, (R*,R*)- (9CI) (CA INDEX NAME)



L12 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

AN 1986:5308 CAPLUS

DN 104:5308

TI Reactions with aziridines. 33. Arene hydrides. Part 1. Highly regioselective ring cleavage of N-acylaziridines by "anthracene hydride" (anion of 9,10-dihydroanthracene). Intermediacy of a carbonyl adduct. Influence of nitrogen inversion on the ring opening

AU Stamm, Helmut; Sommer, Andreas; Woderer, Anton; Wiesert, Wolfgang; Mall, Thomas; Assithianakis, Petros

CS Pharm.-Chem. Inst., Univ. Heidelberg, Heidelberg, D-6900, Fed. Rep. Ger.

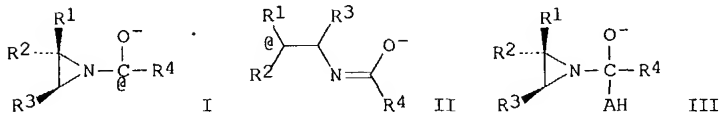
SO Journal of Organic Chemistry (1985), 50(24), 4946-55
CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 104:5308

GI

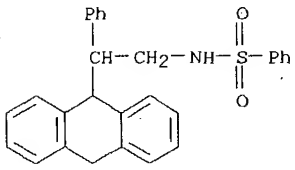


I II III

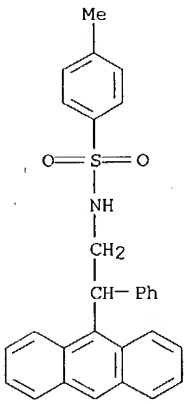
AB Anthracene hydride (AH-) reacts with N-acylaziridines by reductive opening of the aziridine ring and/or amidoethylation of AH-. When the two aziridine carbons are differently substituted, in both reactions only that bond is broken which can form the more stable carbon radical quite in accord with the intermediacy of a radical anion (ketyl) I and with the known homolytic cleavage of I forming the radical II. The extra electron in I is provided by AH- being oxidized to the radical AH•, which can react with II either by radical combination or by hydrogen transfer. The reaction of AH- with N-aroylaziridines can be interrupted at the stage of the carbonyl adduct III as is shown by the isolation of the ketones AHCOR4. Thus, III (R4 = aryl) is considered to be in equilibrium with the radical pair AH•/I. The conversion of III into the final products progresses as expected from its structure apart from the observed retardation by a Ph substituent in the aziridine ring. This retardation is tentatively explained by a hypothesis assuming ring opening of I to occur in the transition state of nitrogen inversion. The anion X- of xanthene resembles AH- in its reactivity. Both carbanions react with N-sulfonylaziridines as expected from an SN2 mechanism.

10690341

IT **98943-90-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 98943-90-9 CAPLUS
CN Benzenesulfonamide, N-[2-(9,10-dihydro-9-anthracenyl)-2-phenylethyl]-
(9CI) (CA INDEX NAME)



L6 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 2001:779961 CAPLUS
DN 136:216604
TI First examples of C-arylation of aziridines catalyzed by indium triflate
AU Yadav, J. S.; Subba Reddy, B. V.; Srinivasa Rao, R.; Veerendhar, G.; Nagaiah, K.
CS Division of Organic Chemistry, Indian Institute of Chemical Technology, Hyderabad, 500007, India
SO Tetrahedron Letters (2001), 42(45), 8067-8070
CODEN: TELEAY; ISSN: 0040-4039
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 136:216604
AB Aziridines react smoothly with arenes in the presence of a catalytic amount of In(OTf)3 at ambient temperature to afford the corresponding β-aryl amine derivs. in excellent yields with high regioselectivity.
IT **402713-08-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of β-aryl amines by regioselective ring opening reaction of N-tosyl aziridines with arenes and indium triflate catalyst)
RN 402713-08-0 CAPLUS
CN Benzenesulfonamide, N-[2-(9-anthracenyl)-2-phenylethyl]-4-methyl- (9CI) (CA INDEX NAME)



RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1999:460387 CAPLUS
DN 131:87724
TI N-Acyl-2,3,3-triphenylpropylamines and analogs useful as anti-inflammatory compounds
IN Scott, Malcolm; Sanfilippo, Pauline J.; Fitzpatrick, Louis; Cardova, Richard F.; Pan, Kevin; Meschino, Joseph; Jetter, Michele
PA Ortho-McNeil Pharmaceutical Corporation, USA
SO PCT Int. Appl., 81 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 9933786	A1	19990708	WO 1998-US27712	19981229
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RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
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	CA 2284468	AA	19990708	CA 1998-2284468	19981229
	AU 9919485	A1	19990719	AU 1999-19485	19981229
	AU 751031	B2	20020808		
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	AT 218536	E	20020615	AT 1998-964321	19981229
	PT 966430	T	20021129	PT 1998-964321	19981229
	ES 2178298	T3	20021216	ES 1998-964321	19981229
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	US 2003171585	A1	20030911	US 2002-298390	20021118
	US 2004082601	A1	20040429	US 2003-690341	20031021
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	US 1998-221254	A	19981228		
	WO 1998-US27712	W	19981229		
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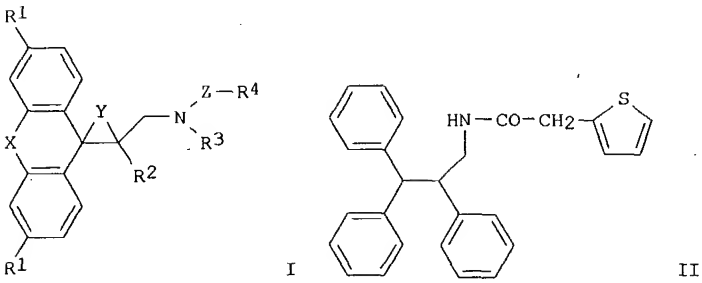
	US 2002-298390	B1	20021118		

OS MARPAT 131:87724

GI



I II

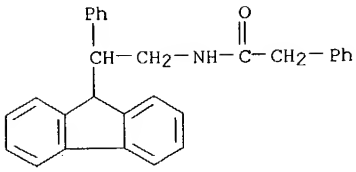
AB Title compds. I [X = single bond, 2H, S, (un)substituted N, (CH2)1-3, CH=CH, or CHxW, where W = O, S, or (un)substituted NH; R1 = 1-3 of C2-C6 alkyl, lower alkoxy, OH, halo, CO2H, etc.; R2 = (un)substituted Ph or heteroarom. ring; Y = CH2 or 2H; R3 = H, (cyclo)alkyl, alkenyl, alkynyl, (un)substituted Ph; Z = CO, CO2, CONH or SO2; R4 = (un)branched C2-C12 alkyl, (un)substituted phenylalkyl or heteroarom. ring], useful as antiinflammatory agents, were prepared The compds. exhibit the beneficial therapeutic properties of glucocorticoids, but may be free of glucocorticoid-like side effects while showing a high affinity for the human glucocorticoid receptor (hGR). Thus, 2-thiopheneacetyl chloride was added to 2,3,3-triphenylpropylamine in ice-cold ClCH2CH2Cl containing NaOAc, and the mixture was stirred overnight at room temperature to afford II. Selected compds. were tested for hGR binding, human progesterone receptor (hPR) binding (side effects), and topical antiinflammatory activity. For instance, II was near equiactive with hydrocortisone in the mouse oxazolone-induced contact hypersensitization (MOCH) assay. The compds. bound selectively to hGR, with IC50 of 7-1500 nM, but showed little or no affinity for hPR.

IT **229972-67-2P 229972-68-3P 229972-69-4P**
229972-70-7P 229972-71-8P 229972-72-9P
229972-73-0P 229972-74-1P 229972-75-2P
229972-76-3P 229972-77-4P 229972-78-5P
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of acyltriphenylpropylamines and analogs as non-steroidal anti-inflammatory agents)

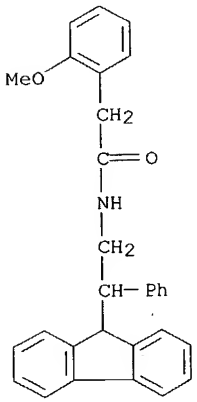
RN 229972-67-2 CAPLUS

CN Benzeneacetamide, N-[2-(9H-fluoren-9-yl)-2-phenylethyl]- (9CI) (CA INDEX

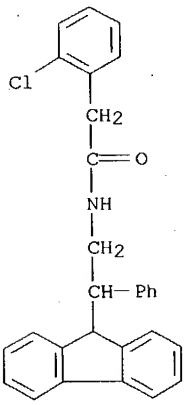
NAME)



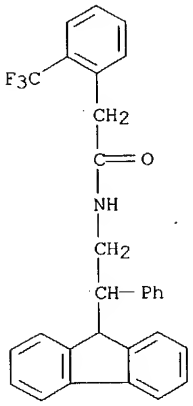
RN 229972-68-3 CAPLUS
CN Benzeneacetamide, N-[2-(9H-fluoren-9-yl)-2-phenylethyl]-2-methoxy- (9CI) (CA INDEX NAME)



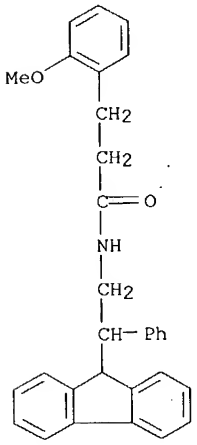
RN 229972-69-4 CAPLUS
CN Benzeneacetamide, 2-chloro-N-[2-(9H-fluoren-9-yl)-2-phenylethyl]- (9CI) (CA INDEX NAME)



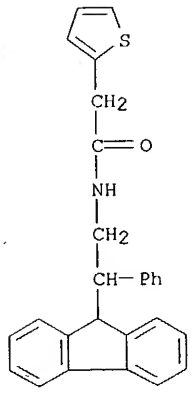
RN 229972-70-7 CAPLUS
CN Benzeneacetamide, N-[2-(9H-fluoren-9-yl)-2-phenylethyl]-2-(trifluoromethyl)- (9CI) (CA INDEX NAME)



RN 229972-71-8 CAPLUS
CN Benzenepropanamide, N-[2-(9H-fluoren-9-yl)-2-phenylethyl]-2-methoxy- (9CI) (CA INDEX NAME)

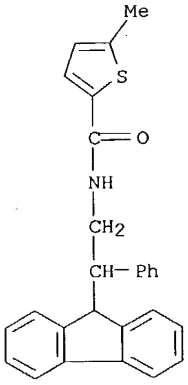


RN 229972-72-9 CAPLUS
CN 2-Thiopheneacetamide, N-[2-(9H-fluoren-9-yl)-2-phenylethyl]- (9CI) (CA INDEX NAME)

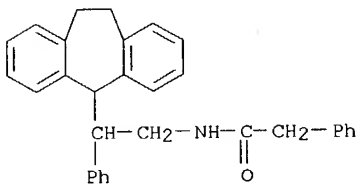


RN 229972-73-0 CAPLUS
CN 2-Thiophenecarboxamide, N-[2-(9H-fluoren-9-yl)-2-phenylethyl]-5-methyl-

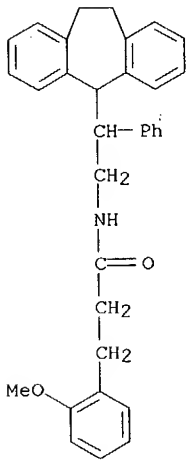
(9CI) (CA INDEX NAME)



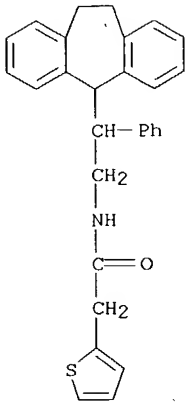
RN 229972-74-1 CAPLUS
CN Benzeneacetamide, N-[2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)-2-phenylethyl]- (9CI) (CA INDEX NAME)



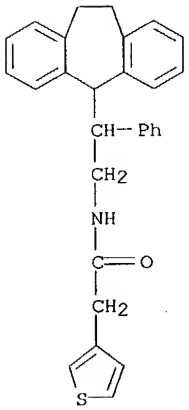
RN 229972-75-2 CAPLUS
CN Benzenepropanamide, N-[2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)-2-phenylethyl]-2-methoxy- (9CI) (CA INDEX NAME)



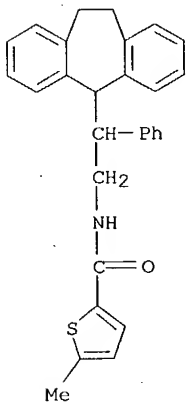
RN 229972-76-3 CAPLUS
CN 2-Thiopheneacetamide, N-[2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)-2-phenylethyl]- (9CI) (CA INDEX NAME)



RN 229972-77-4 CAPLUS
CN 3-Thiopheneacetamide, N-[2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)-2-phenylethyl]- (9CI) (CA INDEX NAME)



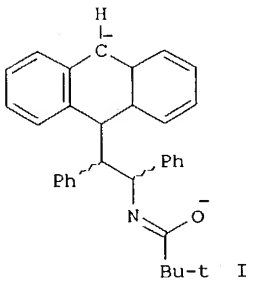
RN 229972-78-5 CAPLUS
CN 2-Thiophenecarboxamide, N-[2-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)-2-phenylethyl]-5-methyl- (9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

10690341

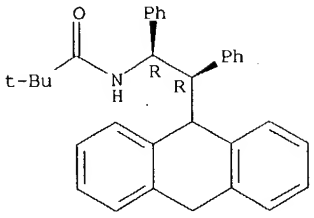
L6 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
AN 1997:773348 CAPLUS
DN 128:75079
TI Electrostatic repulsion by the charged tail of a radical controls the stereochemistry of coupling with anthracenide. Reversibility of benzylic fragmentation
AU Mall, Thomas; Stamm, Helmut
CS Faculty of Pharmacy, University of Heidelberg, Heidelberg, D-69120, Germany
SO Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1997), (11), 2135-2140
CODEN: JCPKBH; ISSN: 0300-9580
PB Royal Society of Chemistry
DT Journal
LA English
GI



I

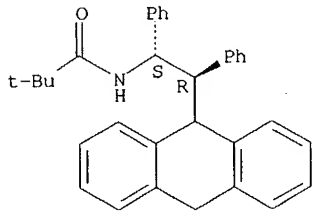
AB Reaction of anthracenide A•- with 1-pivaloyl-2,3-diphenylaziridines cis-4a and trans-4a yields the same products, namely PhCH2CHPhNHCOCMe3 (11) and AH-CHPhCHPhNHCOCMe3 (6) (AH = 9,10-dihydroanthracene-9-yl). The steric differentiation is lost when the two ketyls formed from 4a undergo homolytic ring cleavage forming the same anionic radical PhC•HCHPhN:C(O-)(CMe3) (13). Extremely short reactions (≤10 s) give 6 as the erythro isomer exclusively or nearly so. Coupling of 13 with A•- does not form the precursor (threo-8 = threo-I) of threo-6 owing to electrostatic repulsion between A•- and the anionic tail of 13 in the preferred conformation of the latter. Radical coupling is not completed within this short time so 11 can be formed directly from 13 via PhCH2CHPhN:C(O-)CMe3 (10), the amide enolate anion of 11. Reduction of 13 to carbanion PhC-HCHPhN:C(O-)(CMe3) (9) by outer-sphere electron transfer or via 8 and its benzylic fragmentation (BFR) is the other path to 11. Extending the time to 1 or 2 min has the following effects. Coupling of 13 with A•- is completed at the expense of 11. Second, more than a trace of threo-6 is detected indicating that BFR 8 → 9 + A (A = anthracene) is reversible and that addition of dianion 9 to A proceeds without pronounced stereochem. preference. With even more time the erythro:threo ratio changes in favor of threo-6 and finally can even reach a value slightly less than 1. Simultaneously the amount of 11 increases slowly at the expense of the total 6 indicating that part of BFR which becomes irreversible by carbanion protonation 9 + THF → 10. With much longer reaction times imidate ion 10 eliminates (E)-stilbene. Both isomers of 6 have been independently synthesized from the two isomers of 4a and anthracene hydride AH-.
IT **200569-99-9P 200570-04-3P 200570-11-2P 200570-13-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(electrostatic repulsion by the charged tail of a radical controls the stereochem. of coupling with anthracenide. Reversibility of benzylic fragmentation)
RN 200569-99-9 CAPLUS
CN Propanamide, N-[2-(9,10-dihydro-9-anthracenyl)-1,2-diphenylethyl]-2,2-dimethyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



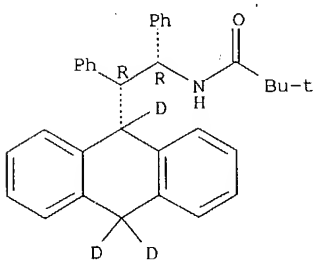
RN 200570-04-3 CAPLUS
CN Propanamide, N-[2-(9,10-dihydro-9-anthracenyl)-1,2-diphenylethyl]-2,2-dimethyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



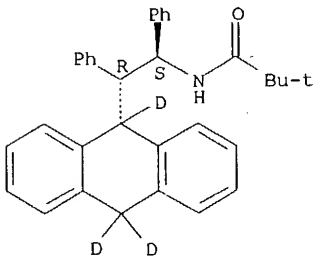
RN 200570-11-2 CAPLUS
CN Propanamide, N-[2-(9,10-dihydro-9,10-d2-9-anthracenyl-10-d)-1,2-diphenylethyl]-2,2-dimethyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 200570-13-4 CAPLUS
CN Propanamide, N-[2-(9,10-dihydro-9,10-d2-9-anthracenyl-10-d)-1,2-diphenylethyl]-2,2-dimethyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

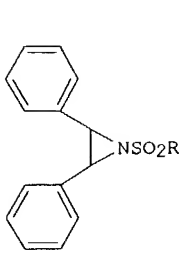


RE.CNT 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

10690341

AN 1996:733731 CAPLUS
DN 126:117781
TI Elimination of stilbene in reactions of sulfonyl-activated stilbene imines
AU Mall, T.; Stamm, H.
CS Fakulty Pharmazy, Univ. Heidelberg, Heidelberg, D-69120, Germany
SO Pharmazie (1996), 51(11), 831-833
CODEN: PHARAT; ISSN: 0031-7144
PB Govi-Verlag Pharmazeutischer Verlag
DT Journal
LA English
GI



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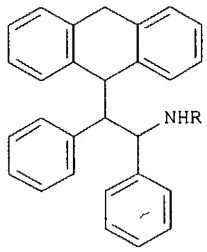


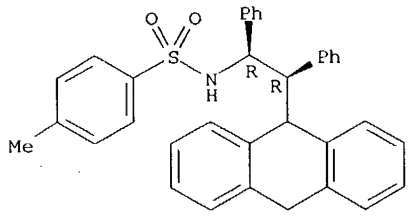
II

AB Anthracene hydride was amidoethylated by sulfonated cis- and trans-stilbene imines I (R = Ph, 4-MeC6H4) yielding the corresponding erythro- and threo-(amidodiphenylethyl)dihydroanthracene II. A benzylic fragmentation yielding PhCH2CHPhNHR was expected as secondary reaction but only trans-stilbene was found. This points to an elimination of RSO2NLi2 (R = Ph, 4-MeC6H4) in the last step of the reaction sequence.

IT **185515-66-6P 185515-67-7P 185515-68-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(elimination of stilbene in reactions of sulfonyl-activated stilbene imines)

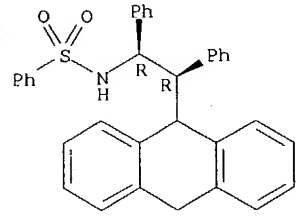
RN 185515-66-6 CAPLUS
CN Benzenesulfonamide, N-[2-(9,10-dihydro-9-anthracenyl)-1,2-diphenylethyl]-4-methyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 185515-67-7 CAPLUS
CN Benzenesulfonamide, N-[2-(9,10-dihydro-9-anthracenyl)-1,2-diphenylethyl]-, (R*,R*)- (9CI) (CA INDEX NAME)

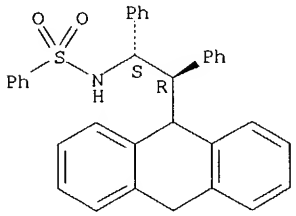
Relative stereochemistry.



10690341

RN 185515-68-8 CAPLUS
CN Benzenesulfonamide, N-[2-(9,10-dihydro-9-anthracenyl)-1,2-diphenylethyl]-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



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